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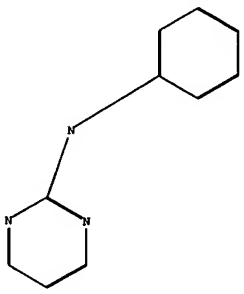

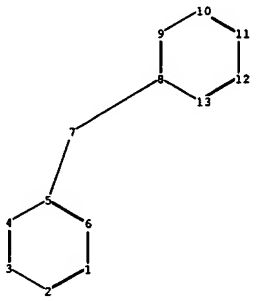

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1 2 3 4 5 6 7 8 9 10 11 12 13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-13 9-10 10-11 11-12 12-13
exact/norm bonds :
5-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom

```
=> d his

     (FILE 'HOME' ENTERED AT 10:17:48 ON 10 FEB 2006)

     FILE 'REGISTRY' ENTERED AT 10:17:53 ON 10 FEB 2006
L1             STRUCTURE UPLOADED
L2               6 S L1
L3             118 S L1 SSS FUL

     FILE 'CAPLUS' ENTERED AT 10:18:23 ON 10 FEB 2006
L4              15 S L3

=> d l1
L1 HAS NO ANSWERS
L1                STR
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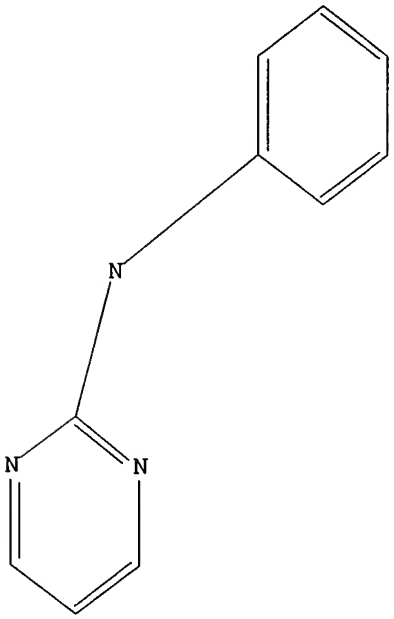


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Structure attributes must be viewed using STN Express query preparation.

=> d ibib abs hitstr total
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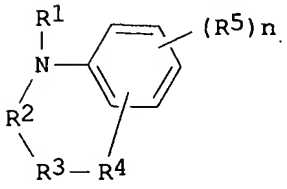
L4 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:756664 CAPLUS
DOCUMENT NUMBER: 141:243576
TITLE: Preparation of macrocycle amino compounds and compositions as cyclin-dependent protein kinase inhibitors
INVENTOR(S): Ren, Pingda; Adrian, Francisco; Gray, Nathanael S.; Wang, Xia
PATENT ASSIGNEE(S): IRM LLC, Bermuda
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078682	A2	20040916	WO 2004-US6947	20040305
WO 2004078682	A3	20051208		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2004235841	A1	20041125	US 2004-794454	20040305
PRIORITY APPLN. INFO.:			US 2003-452633P P	20030305
OTHER SOURCE(S):	MARPAT 141:243576			

GI



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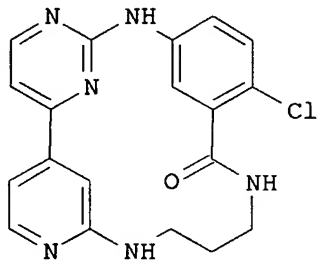


II

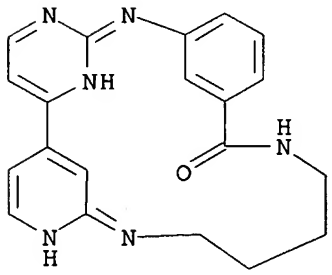
AB The invention provides a novel class of cyclic compds. I, wherein n is 0-3; R1 hydrogen and alkyl; R2-R3 are independently substituted arylene and hetero-arylene; R4 4 is -XIR6(CH2)mNR7C(O)-, -XNR6(CH2)mNR7C(O)CH2-, -XR6(CH2)mNR7(CH2)mNR7C(O)-, -O(CH2)mNR7C(O)-, -NR6(CH2)mO- and -XNR6(CH2)mNR7CH2-; wherein X is a bond or C-alkylene; m is 1-6; R6 and R7 independently are hydrogen and alkyl; and R5 is halo, alkyl, halo-substituted alkyl, alkoxy and halo-substituted alkoxy and

heterocycloalkyl; wherein any heterocycloalkyl of R5 is substituted with a group halo, alkyl, halo-substituted alkyl, alkoxy, halo-substituted alkoxy, heterocycloalkyl-alkyl and -XNR8R9, wherein X is a bond or alkylene; R8 and R9 are independently hydrogen and alkyl; or a salt thereof pharmaceutical compns. comprising such cyclic compds. and methods of using such compds. to treat or prevent diseases and disorders associated with cyclin-dependent kinases (CDKs) activity, particularly diseases associated with the activity of CDK2 and CDK5. Thus, macrocycle II was prepared and tested as CDK2 and CDK5 inhibitors.

IT **752245-04-8P 752245-05-9P 752245-06-0P**
752245-07-1P 752245-08-2P 752245-09-3P
752245-10-6P 752245-11-7P 752245-12-8P
752245-13-9P 752245-14-0P 752245-15-1P
752245-16-2P 752245-17-3P 752245-18-4P
752245-19-5P 752245-20-8P 752245-22-0P
752245-23-1P 752245-24-2P 752245-25-3P
752245-26-4P 752245-27-5P 752245-28-6P
752245-29-7P 752245-30-0P 752245-31-1P
752245-32-2P 752245-36-6P 752245-37-7P
752245-38-8P
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of macrocycle amino compds. and compns. as cyclin-dependent protein kinase inhibitors)

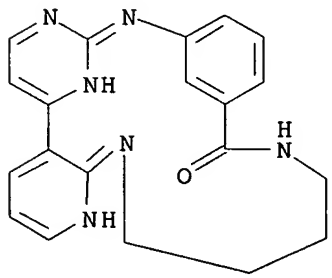
RN 752245-04-8 CAPLUS

CN 5,7,14,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-13-one (9CI) (CA INDEX NAME)

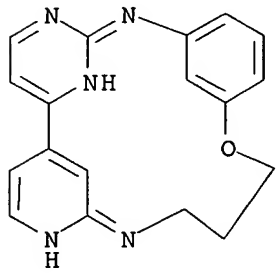


RN 752245-05-9 CAPLUS

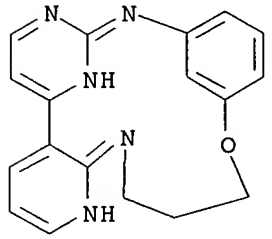
CN 7H,13H-8,12-Metheno-14,18-nitrilopyrido[3,2-g][1,3,9,14]tetraazacycloeicosin-7-one, 1,2,3,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



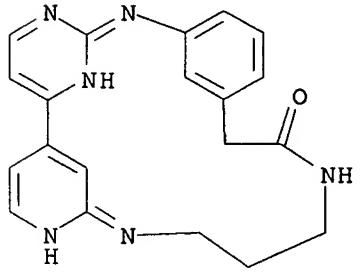
RN 752245-06-0 CAPLUS
CN 13-Oxa-5,7,17,19,24-pentaazatetracyclo[16.3.1.12,6.18,12]tetracosa-1(22),2,4,6(24),8,10,12(23),18,20-nonaene (9CI) (CA INDEX NAME)



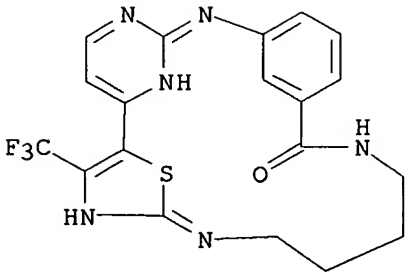
RN 752245-07-1 CAPLUS
CN 11H-6,10-Metheno-12,16-nitrilo-10H-pyrido[2,3-f][1,5,11,13]oxatriazacyclooctadecine, 1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



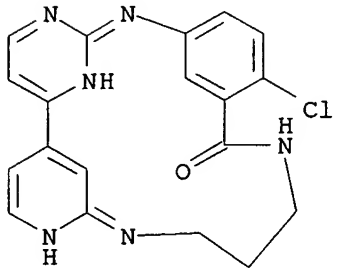
RN 752245-08-2 CAPLUS
CN 5,7,15,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-14-one (9CI) (CA INDEX NAME)



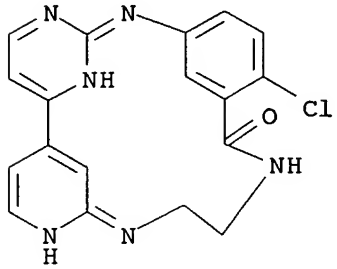
RN 752245-09-3 CAPLUS
CN 25-Thia-4,6,11,18,20,23-hexaazatetracyclo[17.3.1.12,5.113,17]pentacosa-1(22),2,4,13(24),14,16,19,20-octaen-12-one, 3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



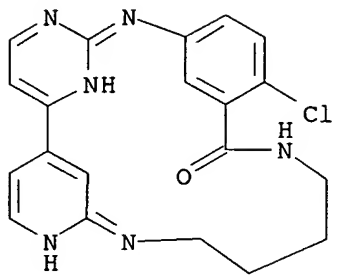
RN 752245-10-6 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one, 11-chloro- (9CI) (CA INDEX NAME)



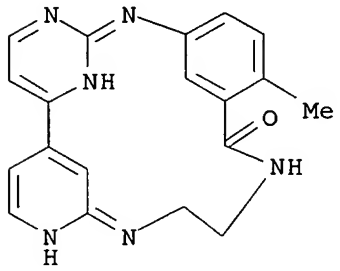
RN 752245-11-7 CAPLUS
CN 5,7,14,17,19,24-Hexaazatetracyclo[16.3.1.12,6.18,12]tetracosa-1(22),2,4,6(24),8,10,12(23),18,20-nonaen-13-one, 11-chloro- (9CI) (CA INDEX NAME)



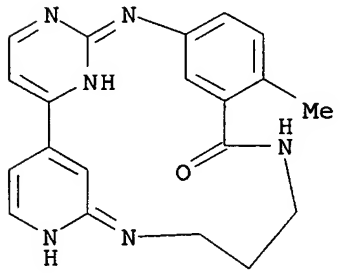
RN 752245-12-8 CAPLUS
CN 5,7,14,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-13-one, 11-chloro- (9CI) (CA INDEX NAME)



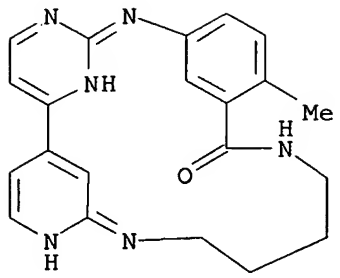
RN 752245-13-9 CAPLUS
CN 5,7,14,17,19,24-Hexaazatetracyclo[16.3.1.12,6.18,12]tetracosa-1(22),2,4,6(24),8,10,12(23),18,20-nonaen-13-one, 11-methyl- (9CI) (CA INDEX NAME)



RN 752245-14-0 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one, 11-methyl- (9CI) (CA INDEX NAME)



RN 752245-15-1 CAPLUS
CN 5,7,14,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-13-one, 11-methyl- (9CI) (CA INDEX NAME)



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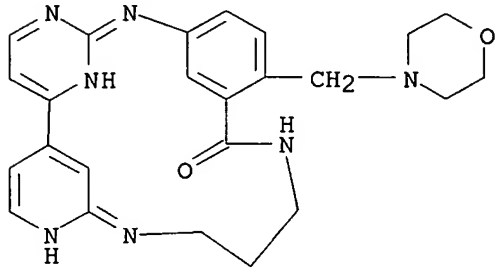
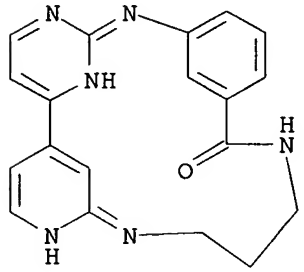
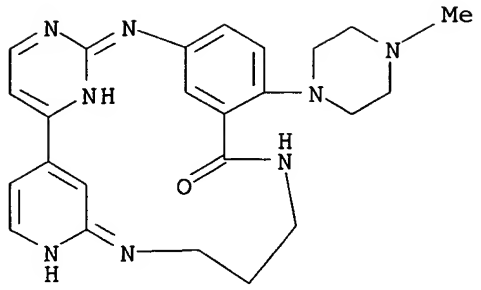
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one, 11-(4-morpholinylmethyl)- (9CI) (CA INDEX NAME)



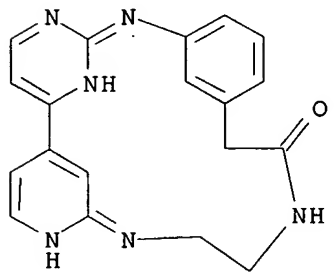
RN 752245-17-3 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one (9CI) (CA INDEX NAME)



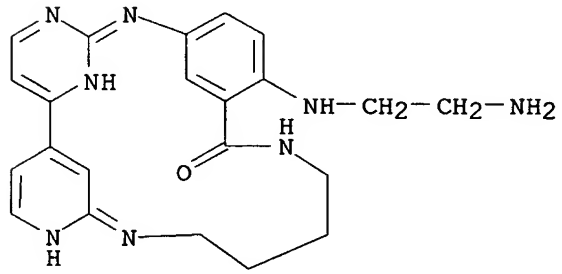
RN 752245-18-4 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one, 11-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



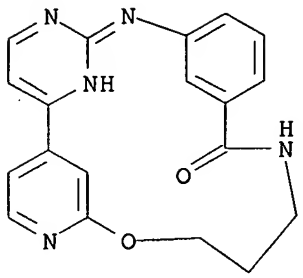
RN 752245-19-5 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-14-one (9CI) (CA INDEX NAME)



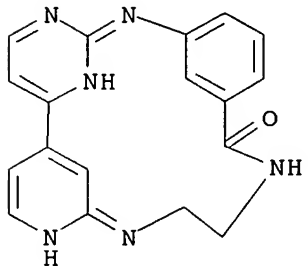
RN 752245-20-8 CAPLUS
CN 5,7,14,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-13-one, 11-[(2-aminoethyl)amino]- (9CI) (CA INDEX NAME)



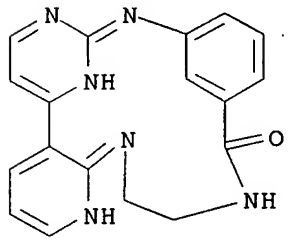
RN 752245-22-0 CAPLUS
CN 18-Oxa-5,7,14,20,25-pentaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaen-13-one (9CI) (CA INDEX NAME)



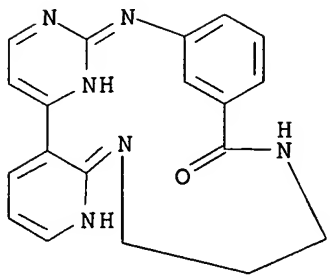
RN 752245-23-1 CAPLUS
CN 5,7,14,17,19,24-Hexaazatetracyclo[16.3.1.12,6.18,12]tetracosa-1(22),2,4,6(24),8,10,12(23),18,20-nonaen-13-one (9CI) (CA INDEX NAME)



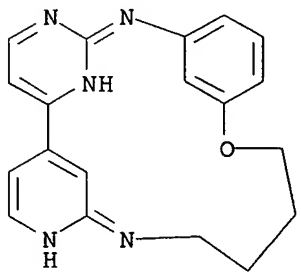
RN 752245-24-2 CAPLUS
CN 5H,11H-6,10-Metheno-12,16-nitrilopyrido[3,2-g][1,3,9,12]tetraazacyclooctadecin-5-one, 1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)



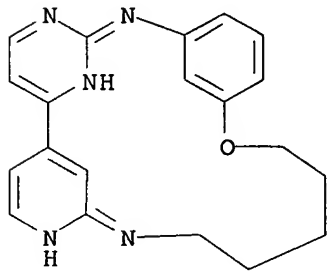
RN 752245-25-3 CAPLUS
CN 7,11-Metheno-13,17-nitrilo-12H-pyrido[3,2-g][1,3,9,13]tetraazacyclononadecin-6(1H)-one, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



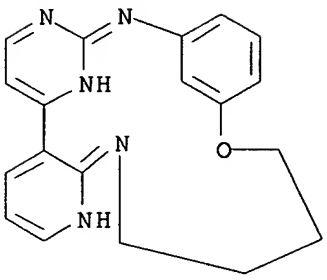
RN 752245-26-4 CAPLUS
CN 13-Oxa-5,7,18,20,25-pentaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaene (9CI) (CA INDEX NAME)



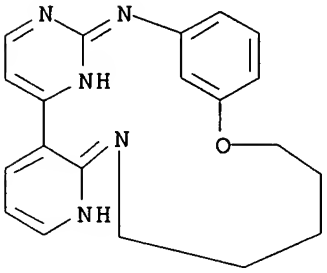
RN 752245-27-5 CAPLUS
CN 13-Oxa-5,7,19,21,26-pentaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaene (9CI) (CA INDEX NAME)



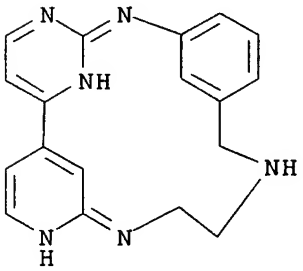
RN 752245-28-6 CAPLUS
CN 1H,12H-7,11-Metheno-13,17-nitrilopyrido[2,3-g][1,6,12,14]oxatriazacyclononadecine, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



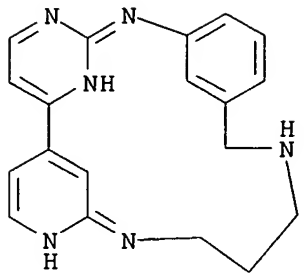
RN 752245-29-7 CAPLUS
CN 13H-8,12-Metheno-14,18-nitrilo-12H-pyrido[3,2-m][1,7,9,15]oxatriazacycloeicosine, 1,2,3,4,5,6-hexahydro- (9CI) (CA INDEX NAME)



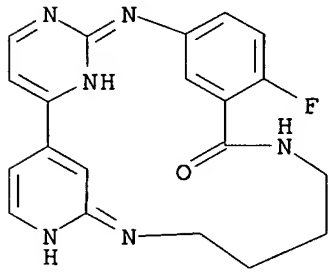
RN 752245-30-0 CAPLUS
CN 5,7,14,17,19,24-Hexaazatetracyclo[16.3.1.12,6.18,12]tetracosa-1(22),2,4,6(24),8,10,12(23),18,20-nonaene (9CI) (CA INDEX NAME)



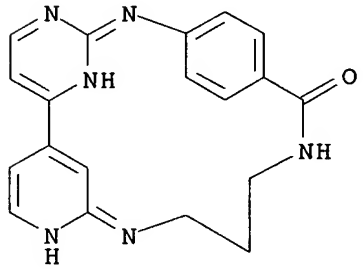
RN 752245-31-1 CAPLUS
CN 5,7,14,18,20,25-Hexaazatetracyclo[17.3.1.12,6.18,12]pentacosa-1(23),2,4,6(25),8,10,12(24),19,21-nonaene (9CI) (CA INDEX NAME)



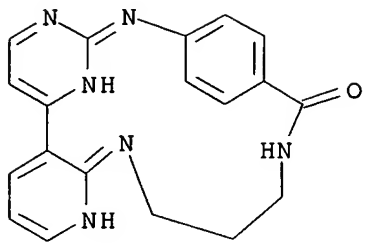
RN 752245-32-2 CAPLUS
CN 5,7,14,19,21,26-Hexaazatetracyclo[18.3.1.12,6.18,12]hexacosa-1(24),2,4,6(26),8,10,12(25),20,22-nonaen-13-one, 11-fluoro- (9CI) (CA INDEX NAME)



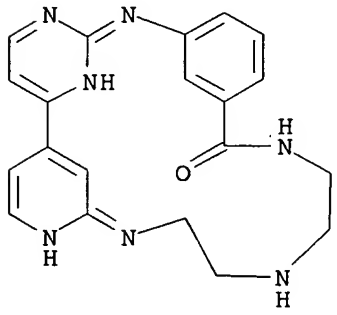
RN 752245-36-6 CAPLUS
CN 2,4,11,13,17,25-Hexaazatetracyclo[17.2.2.13,7.18,12]pentacosa-1(21),3,5,7(25),8,10,12(24),19,22-nonaen-18-one (9CI) (CA INDEX NAME)



RN 752245-37-7 CAPLUS
CN 1H-7,10-Etheno-12,16-nitrilopyrido[3,2-g][1,3,9,13]tetraazacyclooctadecin-6(11H)-one, 2,3,4,5-tetrahydro- (9CI) (CA INDEX NAME)



RN 752245-38-8 CAPLUS
CN 5,7,14,17,20,22,27-Heptaazatetracyclo[19.3.1.12,6.18,12]heptacosa-1(25),2,4,6(27),8,10,12(26),21,23-nonaen-13-one (9CI) (CA INDEX NAME)



applicant

L4 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:177944 CAPLUS
DOCUMENT NUMBER: 140:235737
TITLE: Production of macrocyclic pyrimidine derivatives and their use as drugs
INVENTOR(S): Luecking, Ulrich; Siemeister, Gerhard; Schaefer, Martina; Briem, Hans
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 42 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10239042	A1	20040304	DE 2002-10239042	20020821
CA 2492319	AA	20040401	CA 2003-2492319	20030805
WO 2004026881	A1	20040401	WO 2003-EP8664	20030805
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1530574	A1	20050518	EP 2003-797225	20030805
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003012874	A	20050628	BR 2003-12874	20030805
JP 2006501271	T2	20060112	JP 2004-536924	20030805
US 2004209895	A1	20041021	US 2003-644076	20030820
NO 2005001448	A	20050318	NO 2005-1448	20050318

PRIORITY APPLN. INFO.:
DE 2002-10239042 A 20020821
US 2002-413444P P 20020926
WO 2003-EP8664 W 20030805

OTHER SOURCE(S): CASREACT 140:235737; MARPAT 140:235737
GI

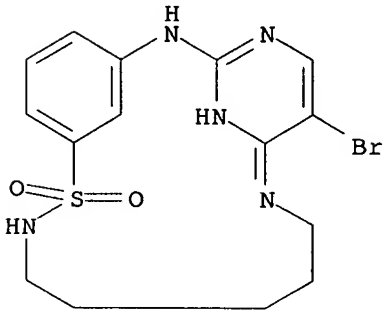
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Macrocyclic pyrimidine derivs., e.g., I [R1, R5 = H, OH, halogen, NO2, CN, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heteroaryl, etc.; R2 = H, C1-10-alkyl; R3 = H, halogen, NO2, CN, C1-10-alkyl, C1-10-haloalkyl, C2-10-alkenyl, C2-10-alkynyl, C2-10-cycloalkyl, OH, C1-6-alkoxy, C1-6-alkylthio, NH2, NH(CH2)p-C3-10-cycloalkyl, C1-6-hydroxyalkyl, (C1-6-alkoxy)-(C1-6-alkyl), NH(C1-6-alkyl), N(C1-6-alkyl)2, SO(C1-6-alkyl), SO2(C1-6-alkyl), (C1-6-alkanoyl), CONR8R9, COR10, (C1-6-alkyl)-OAc, CO2H, aryl, heteroaryl, etc.; R4 = H, halogen, C1-4-alkyl; R6, R7, R8, R9, R10, R11 = H, OH, halogen, C1-12-alkoxy, C1-6-alkylthio, NH2, CN, C1-6-alkyl, NH(CH2)p-C3-10-cycloalkyl,

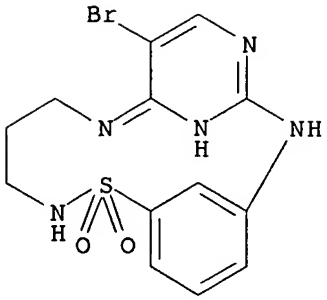
C3-10-cycloalkyl, C1-6-hydroxyalkyl, C2-6-alkenyl, C2-6-alkynyl, NH-(C1-6-alkyl), N(C1-6-alkyl)2, SO(C1-6-alkyl), SO2(C1-6-alkyl), C1-6-alkanoyl, CONR8R9, etc.; X, Y = O, S, NR11, NR11O, ONR11, CR6R7, C:O, C:S, SO, SO2, C(:O)O, OC(:O), S(:O)O, OS(:O), SO2-O, O-SO2, CONR8, NR8CO, OC(:O)NR8, NR8C(:O)O, CSNR8, NR8CS, OC(:S)NR8, SONR8, NR8SO, SO2NR8, NR8SO2, NR8COR9, NR8CSNR9, NR8SONR9, NR8SO2NR9, NR8CONR9, NR8CSNR9; A = aryl, heteroaryl; B = bond ; m = 0 - 8; n, p = 0 - 6], II (D = NH2, NO2) and III (U = OH), their isomers, stereoisomers, enantiomers and their salts, which are inhibitors of the cyclin-dependent kinases, procedures for their production as well as their use as medicine for the treatment of different illnesses is described. Preparation of I is characterized by macrocyclization of pyrimidine IV (L = leaving group) in the presence of an acid and is itself prepared via reduction of nitro compound V (L = leaving group). Thus, I [R1 = R2 = R4 = R5 = H, R3 = Br, A = 1,3-phenylene, (Y)nB(X)n = NH(CH2)5NHSO2, m = n = 1] was prepared via macrocyclization of IV [L = Cl, R1 = R2 = R4 = R5 = H, R3 = Br, A = 1,3-phenylene, (Y)nB(X)n = NH(CH2)5NHSO2, m = n = 1]. The inhibitory activity of I [R1 = R2 = R4 = R5 = H, R3 = Br, A = 1,3-phenylene, (Y)nB(X)n = NH(CH2)5NHSO2, m = n = 1] towards cyclin-dependent kinases was determined [IC50 = 420 nM vs. CDK1/CycB, IC50 = 200 nM vs. CDK2/CycE, IC50 = 1.1 nM vs. MCF7].

IT **666719-26-2P 666719-27-3P 666719-28-4P**
666719-29-5P 666719-30-8P 666719-32-0P
666719-34-2P 666719-35-3P 666719-36-4P
666719-37-5P 666719-38-6P 666719-39-7P
666719-40-0P 666719-41-1P 666719-42-2P
666719-43-3P 666719-44-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of macrocyclic pyrimidine derivs. which are inhibitors of the cyclin-dependent kinases)

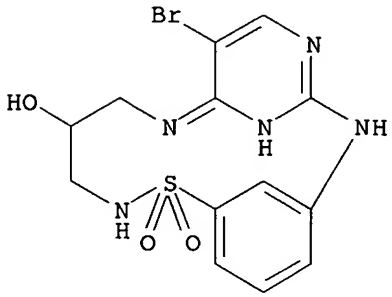
RN 666719-26-2 CAPLUS
CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene, 6-bromo-, 15,15-dioxide (9CI) (CA INDEX NAME)



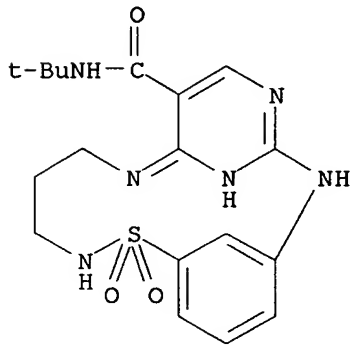
RN 666719-27-3 CAPLUS
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo-, 13,13-dioxide (9CI) (CA INDEX NAME)



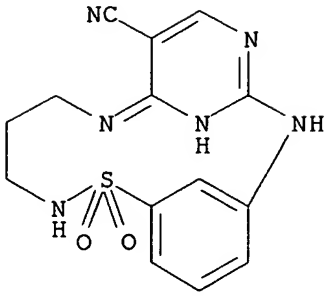
RN 666719-28-4 CAPLUS
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaen-10-ol, 6-bromo-, 13,13-dioxide (9CI) (CA INDEX NAME)



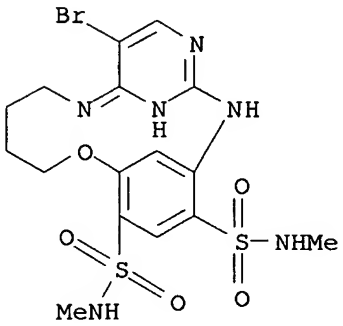
RN 666719-29-5 CAPLUS
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene-6-carboxamide, N-(1,1-dimethylethyl)-, 13,13-dioxide (9CI) (CA INDEX NAME)



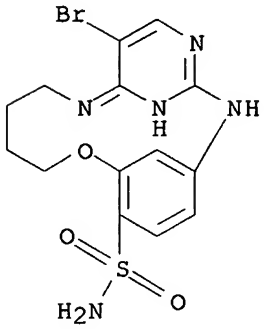
RN 666719-30-8 CAPLUS
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene-6-carbonitrile, 13,13-dioxide (9CI) (CA INDEX NAME)



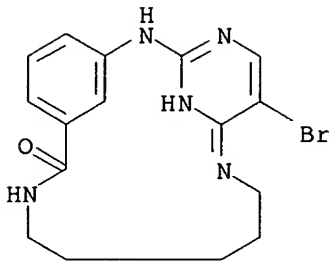
RN 666719-32-0 CAPLUS
CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),3,5,7(19),14,16-hexadecaene-15,17-disulfonamide, 6-bromo-N,N'-dimethyl- (9CI) (CA INDEX NAME)



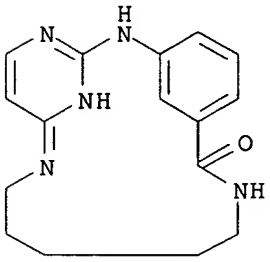
RN 666719-34-2 CAPLUS
CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene-15-sulfonamide, 6-bromo- (9CI) (CA INDEX NAME)



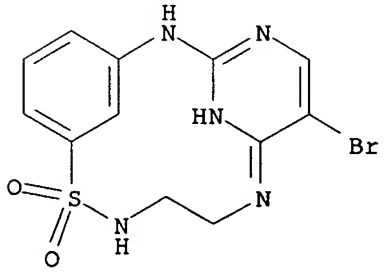
RN 666719-35-3 CAPLUS
CN 2,4,8,14,21-Pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaen-15-one, 6-bromo- (9CI) (CA INDEX NAME)



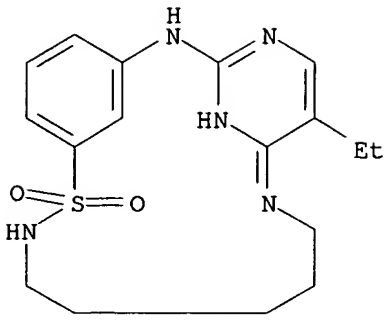
RN 666719-36-4 CAPLUS
CN 2,4,8,14,21-Pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaen-15-one (9CI) (CA INDEX NAME)



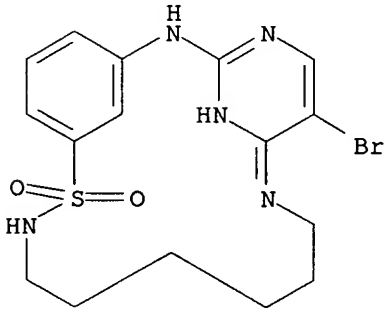
RN 666719-37-5 CAPLUS
CN 12-Thia-2,4,8,11,18-pentaazatricyclo[11.3.1.13,7]octadeca-1(17),2,4,6,13,15-hexaene, 6-bromo-, 12,12-dioxide (9CI) (CA INDEX NAME)



RN 666719-38-6 CAPLUS
CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene, 6-ethyl-, 15,15-dioxide (9CI) (CA INDEX NAME)

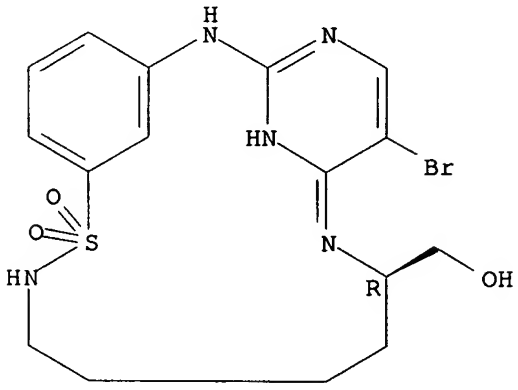


RN 666719-39-7 CAPLUS
CN 16-Thia-2,4,8,15,22-pentaazatricyclo[15.3.1.13,7]docosa-1(21),2,4,6,17,19-hexaene, 6-bromo-, 16,16-dioxide (9CI) (CA INDEX NAME)

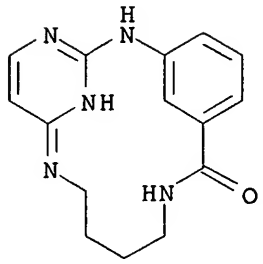


RN 666719-40-0 CAPLUS
CN 15-Thia-2,4,8,14,21-pentaazatricyclo[14.3.1.13,7]heneicosa-1(20),2,4,6,16,18-hexaene-9-methanol, 6-bromo-, 15,15-dioxide, (9R)- (9CI) (CA INDEX NAME)

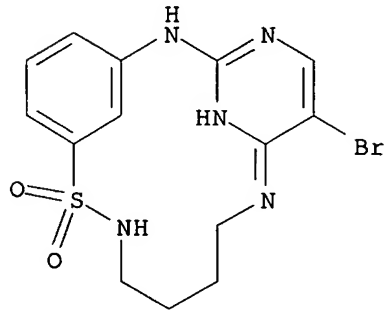
Absolute stereochemistry.



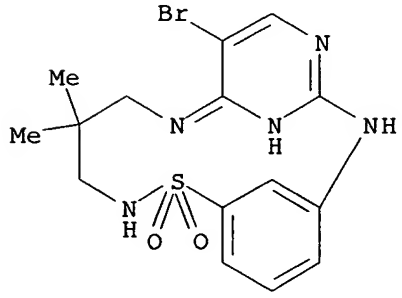
RN 666719-41-1 CAPLUS
CN 2,4,8,13,20-Pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaen-14-one (9CI) (CA INDEX NAME)



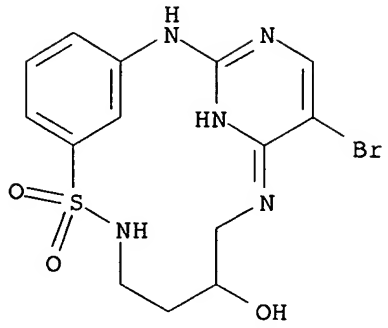
RN 666719-42-2 CAPLUS
CN 14-Thia-2,4,8,13,20-pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaene, 6-bromo-, 14,14-dioxide (9CI) (CA INDEX NAME)



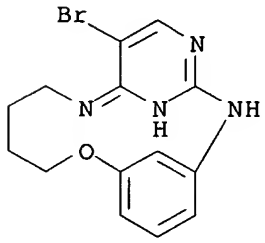
RN 666719-43-3 CAPLUS
CN 13-Thia-2,4,8,12,19-pentaazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo-10,10-dimethyl-, 13,13-dioxide (9CI) (CA INDEX NAME)



RN 666719-44-4 CAPLUS
CN 14-Thia-2,4,8,13,20-pentaazatricyclo[13.3.1.13,7]eicosa-1(19),2,4,6,15,17-hexaen-10-ol, 6-bromo-, 14,14-dioxide (9CI) (CA INDEX NAME)



IT **666719-33-1P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, aminosulfonylation and inhibition by, of cyclin-dependent kinases; preparation of macrocyclic pyrimidine derivs. which are inhibitors of the cyclin-dependent kinases)
RN 666719-33-1 CAPLUS
CN 13-Oxa-2,4,8,19-tetraazatricyclo[12.3.1.13,7]nonadeca-1(18),2,4,6,14,16-hexaene, 6-bromo- (9CI) (CA INDEX NAME)

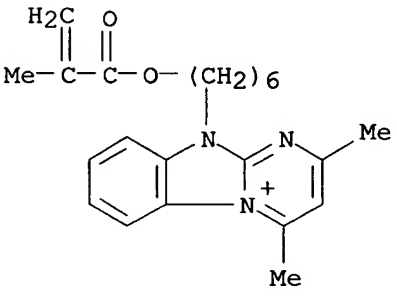


L4 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:737797 CAPLUS
DOCUMENT NUMBER: 132:85803
TITLE: Light-sensitive methacrylic acid based copolymers containing the 2-(2-chloroanilino)-4,6-dimethylpyrimidine chromophore in the side chain
AUTHOR(S): Lebedeva, G. K.; Ivanova, V. N.; Denisov, V. M.; Kudryavtsev, V. V.; Frolov, A. N.
CORPORATE SOURCE: Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg, Russia
SOURCE: Russian Journal of General Chemistry (Translation of Zhurnal Obshchei Khimii) (1999), 69(6), 981-985
CODEN: RJGCEK; ISSN: 1070-3632
PUBLISHER: MAIK Nauka/Interperiodica Publishing
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New light-sensitive copolymers containing the o-chlorophenylpyrimidine chromophore in the side chain were prepared and studied. The 1H NMR and electronic spectra, interpreted using model compds., showed that the main photochem. reaction of the copolymers is cyclization at the heterocyclic nitrogen atom of the o-chloropyrimidinium chromophore to give N-substituted pyrimido[1,2-a]benzimidazolium chromophore.

IT **253662-25-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(photoproduct; photolysis of (dimethylpyrimidyl)(chlorophenyl)aminohexyl methacrylate in relation to photolysis of methacrylate copolymers containing chlorophenylpyrimidine chromophore in side chain)

RN 253662-25-8 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-dimethyl-10-[6-[(2-methyl-1-oxo-2-propenyl)oxy]hexyl]-, chloride (9CI) (CA INDEX NAME)



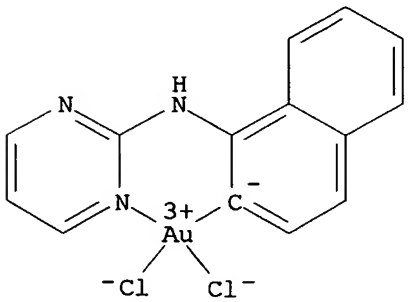
● Cl⁻

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:570215 CAPLUS
DOCUMENT NUMBER: 131:322704
TITLE: Direct cycloauration of 1-(2-pyridylamino and 2-pyrimidinylamino)naphthalene and 2-(p-toluidino)quinoline with sodium tetrachloroaurate(III)
AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Nagoya, 464-8602, Japan
SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands) (1999), 24(4), 449-453
CODEN: TMCHDN; ISSN: 0340-4285
PUBLISHER: Kluwer Academic Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

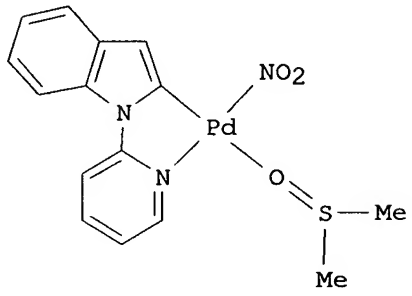
AB 1-(2-Pyridylamino and 2-pyrimidinylamino)naphthalene (abbreviated as Hpyn and Hpmn, resp.) and 2-(p-toluidino)quinoline (Htlq) were directly cycloaurated with Na[AuCl4] to give [AuCl2L] (L = pyn, pmn, or tlq). These complexes were characterized spectroscopically and the square planar structure of [AuCl2(pmn)] was determined by x-ray anal. The naphthalene ring was aurated at position 2, forming a six-membered auraheterocycle with concomitant coordination of the pyrimidine-N atom. The trans influence of the C donor was clearly reflected in the AuCl bond lengths; 2.372(2) trans to C and 2.275 A trans to N. Similar square planar structures were suggested for the other two complexes.

IT **248937-34-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure)
RN 248937-34-0 CAPLUS
CN Gold, dichloro[1-[(2-pyrimidinyl-κN1)amino]-2-naphthalenyl-κC]-, (SP-4-3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:76937 CAPLUS
DOCUMENT NUMBER: 130:223399
TITLE: Cyclometallation of 2-(2-pyridyl)benzo[b]furan and 1-(2-pyridyl and 2-pyrimidyl)indole with palladium(II) and rhodium(III). Structures of unexpectedly formed nitro palladium(II) complexes
AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Nagoya, 464-8602, Japan
SOURCE: Polyhedron (1998), Volume Date 1999, 18(3-4), 533-543
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:223399
GI



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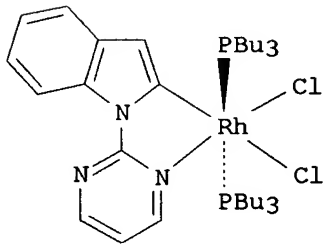


II

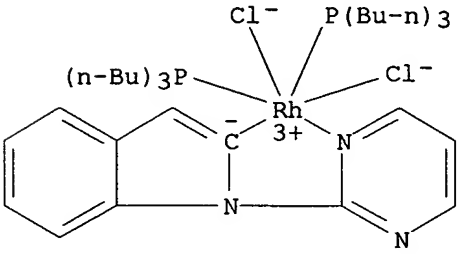
AB Reactions of 2-(2-pyridyl)benzo[b]furan (Hpbf), 1-(2-pyridyl)indole (Hpyi) and 1-(2-pyrimidyl)indole (Hpmi) with palladium(II) acetate in refluxing acetonitrile resulted in the formation of unexpected nitro complexes, [Pd(NO2)L(CH3CN)] (L = pbf, pyi and pmi). The presence of NO2 in the square planar DMSO (DMSO) derivs., [Pd(NO2)L(DMSO)] (L = pbf and pyi I) were confirmed by X-ray anal. Palladation occurred at the C-3 of pbf and at the C-2 of pyi and pmi and a five member palladacycle was formed. The NO2 was coordinated trans to the pyridine-N atom and the DMSO trans to the C atom through the O atom. Cyclorhodation of Hpbf, Hpyi and Hpmi with

trichlorobis(tri-n-butylphosphine)rhodium(III) similarly occurred in refluxing toluene to afford octahedral complexes, [RhCl2L(PBu3)2], (PBu3 = tri-n-butylphosphine). The octahedral structure of [RhCl2(pmi)(PBu3)2] II was also determined by X-ray anal. The two PBu3 ligands were coordinated trans to each other and the strong trans influence of the σ-C donor atom stretched one Rh-Cl bond trans to it.

IT **221043-97-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 221043-97-6 CAPLUS

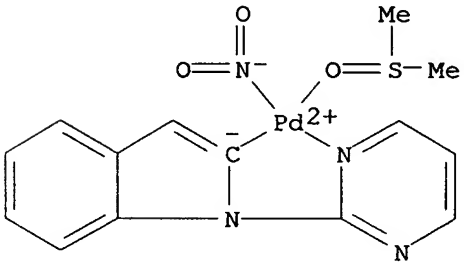
CN Rhodium, dichloro[1-(2-pyrimidinyl-κN1)-1H-indol-2-yl-κC]bis(tributylphosphine)-, (OC-6-43)- (9CI) (CA INDEX NAME)



IT **221044-00-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 221044-00-4 CAPLUS

CN Palladium, (nitrito-κN)[1-(2-pyrimidinyl-κN1)-1H-indol-2-yl-κC][(sulfinyl-κO)bis[methane]]-, (SP-4-4)- (9CI) (CA INDEX NAME)



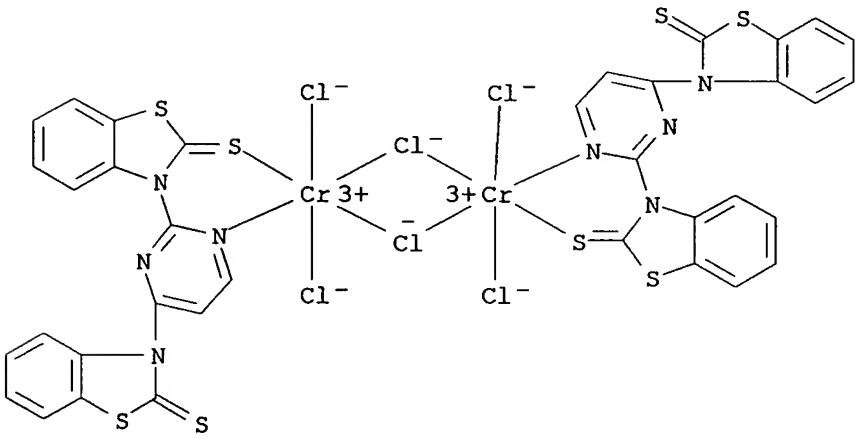
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:316605 CAPLUS
DOCUMENT NUMBER: 129:35688
TITLE: Synthesis and characterization of Mn(II), Co(II), Ni(II), Cu(II), Zn(II), Cr(III), Fe(III), Ru(III) and Rh(III) complexes with 1,1'-(2,6-pyrimidinediyl)bis(benzothiazole-2-thione)
AUTHOR(S): Khan, Tabrez A.; Shahjahan; Zaidi, S. A. A.
CORPORATE SOURCE: Dep. Chemistry, Jamia Millia Islamia, New Delhi, 110 025, India
SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (1998), 37A(2), 161-164
CODEN: ICACEC; ISSN: 0376-4710
PUBLISHER: National Institute of Science Communication, CSIR
DOCUMENT TYPE: Journal
LANGUAGE: English

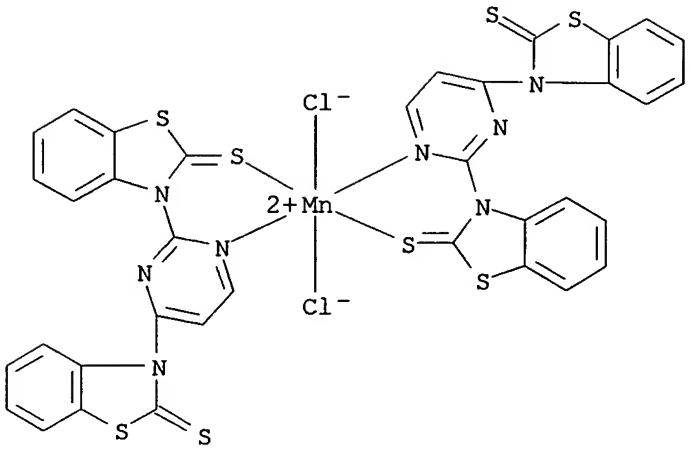
AB M(PBT)2Cl2 and M'2(PBT)2Cl6 (PBT = 1,1'-(2,6-pyrimidinediyl)bis(benzothiazole-2-thione); M = Mn, Co, Ni, Cu, Zn and M' = Cr, Fe, Ru, Rh) were synthesized and characterized by elemental anal., magnetic susceptibility, IR, 1H NMR and electronic spectral studies. The ligand coordinates through pyrimidine N and thiocarbonyl S atoms of the mercaptobenzothiazolyl group. M(PBT)2Cl2 complexes appear to be octahedral whereas M'2(PBT)2Cl6 complexes probably have a Cl-bridged dimeric octahedral structure.

IT **208044-98-8P 208044-99-9P 208045-00-5P**
208045-01-6P 208045-02-7P 208045-03-8P
208045-04-9P 208045-05-0P 208045-06-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

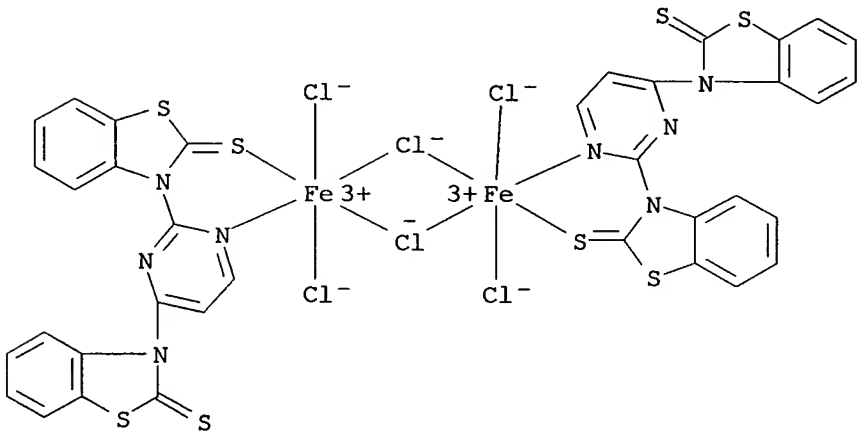
RN 208044-98-8 CAPLUS
CN Chromium, di-μ-chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



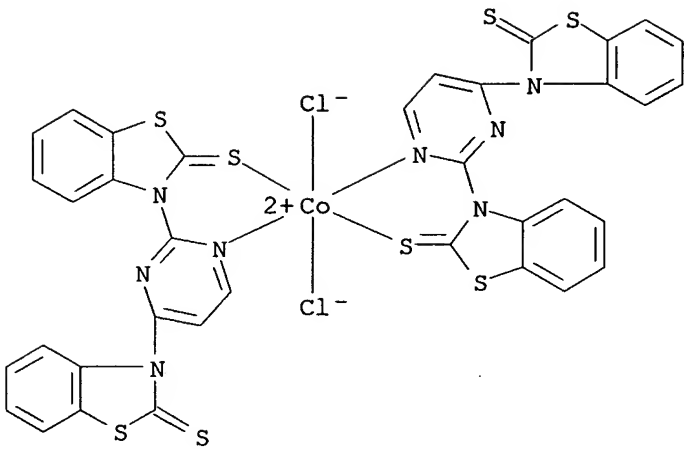
RN 208044-99-9 CAPLUS
CN Manganese, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



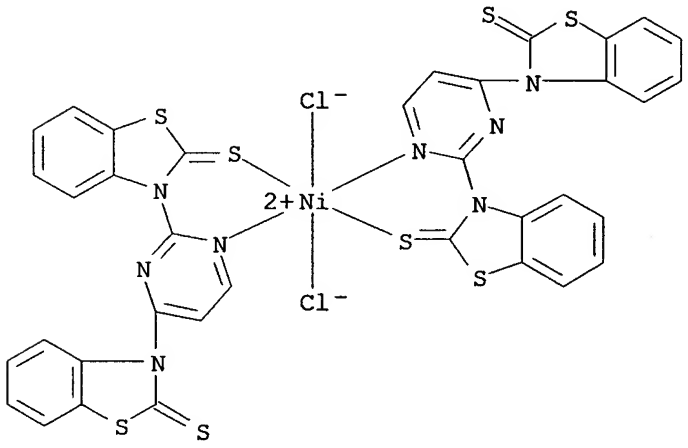
RN 208045-00-5 CAPLUS
CN Iron, di-μ-chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



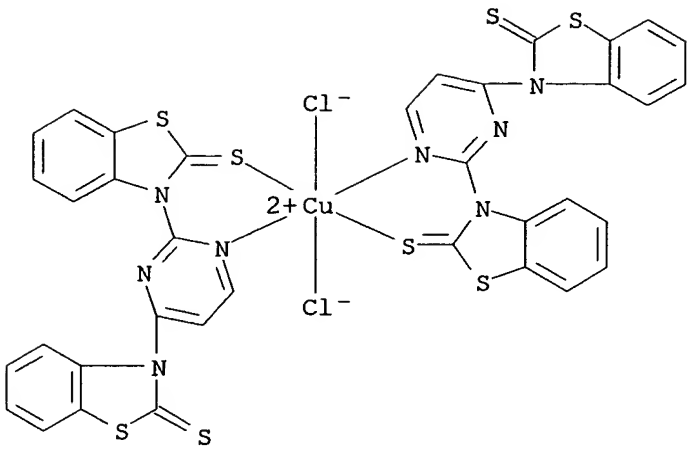
RN 208045-01-6 CAPLUS
CN Cobalt, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



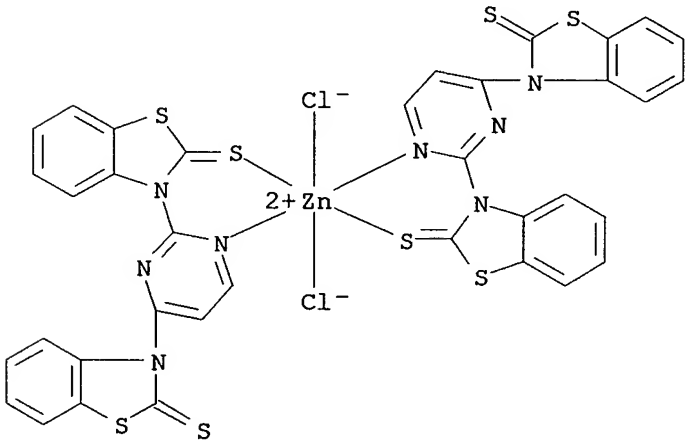
RN 208045-02-7 CAPLUS
CN Nickel, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



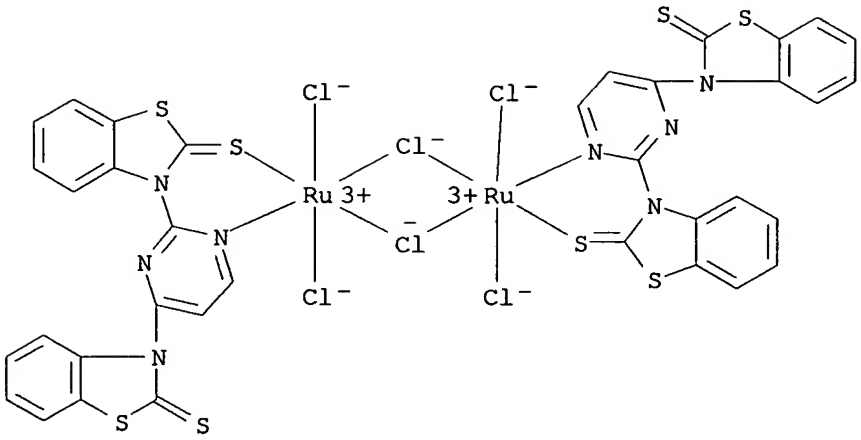
RN 208045-03-8 CAPLUS
CN Copper, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



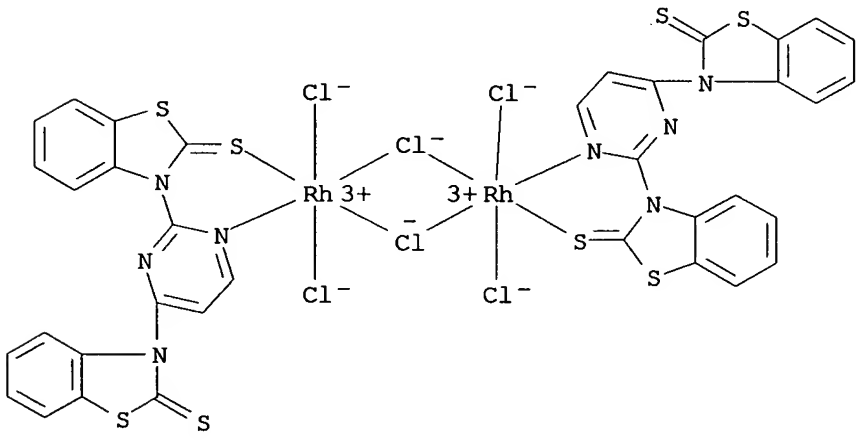
RN 208045-04-9 CAPLUS
CN Zinc, dichlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



RN 208045-05-0 CAPLUS
CN Ruthenium, di-μ-chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)

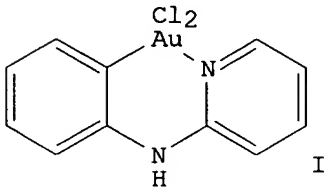


RN 208045-06-1 CAPLUS
CN Rhodium, di-μ-chlorotetrachlorobis[3-[4-(2-thioxo-3(2H)-benzothiazolyl)-2-pyrimidinyl-κN1]-2(3H)-benzothiazolethione-κS2]di- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:707745 CAPLUS
DOCUMENT NUMBER: 128:3751
TITLE: Direct cycloauration of 2-anilinopyridine (Hanp) with tetrachloroaurate(III) and the X-ray crystal structure of [AuCl2(anp)]
AUTHOR(S): Nonoyama, Matsuo; Nakajima, Kiyohiko; Nonoyama, Kiyoko
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Nagoya University, Chikusa, 464-01, Japan
SOURCE: Polyhedron (1997), 16(23), 4039-4044
CODEN: PLYHDE; ISSN: 0277-5387
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:3751
GI

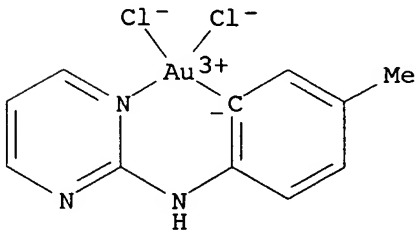


I

AB 2-Anilinopyridine (Hanp) reacted with Na tetrachloroaurate(III) in refluxing H2O directly to give cyclometalated [AuCl2(anp)] I, which was characterized spectroscopically and its structure determined by x-ray anal. The metalation reaction involved direct activation of an ortho C-H bond of the Ph moiety and the deprotonated anionic ligand, anp, coordinated to Au through the pyridine-N and Ph ortho-C atoms forming a six-membered chelate ring. Similarly cycloaurated complexes, [AuBr2(anp)] and [AuCl2(C-N)] (CN = tlp, map, and tpm), were also prepared and characterized [Htlp = 2-(p-toluidino)pyridine, Hmap = 2-(N-methylanilino)pyridine, and Htpm = 2-(p-toluidino)pyrimidine].

IT **198711-23-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(direct cycloauration of anilinopyridine and related compds. with tetrachloroaurate)

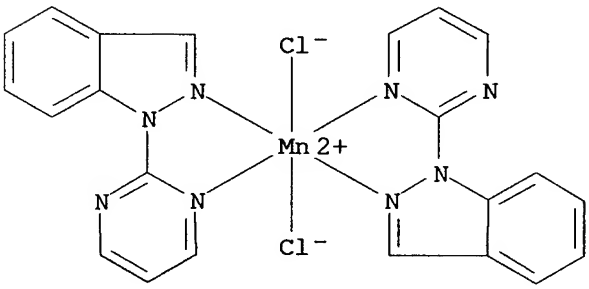
RN 198711-23-8 CAPLUS
CN Gold, dichloro[5-methyl-2-[(2-pyrimidinyl-κN1)amino]phenyl-κC]-, (SP-4-3)- (9CI) (CA INDEX NAME)



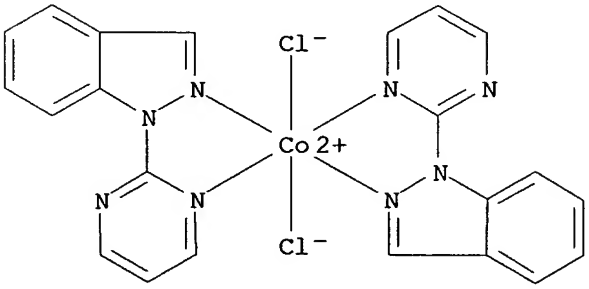
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:419210 CAPLUS
DOCUMENT NUMBER: 119:19210
TITLE: Coordination properties of new indazole derivatives
AUTHOR(S): Zaidi, Saiyid Aftab Ahmad; Shahjahan; Siddiqui, Khwaja Salahuddin
CORPORATE SOURCE: Dep. Chem., Aligarh Muslim Univ., Aligarh, 202 002, India
SOURCE: Transition Metal Chemistry (Dordrecht, Netherlands) (1993), 18(1), 51-4
CODEN: TMCHDN; ISSN: 0340-4285
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The bidentate N donor ligands (L) 2-(1-indazolyl)pyridine and 2-(1-indazolyl)pyrimidine were synthesized. ML2Cl2 (M = Mn, Co, Ni, Cu, Zn) were prepared and characterized by elemental anal., IR, UV spectra, and magnetic susceptibilities. The complexes are nonelectrolytes and have magnetic moments consistent with an octahedral environment.
IT **148099-98-3P 148099-99-4P 148100-20-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR and UV spectra and crystal field parameters and reaction of, with pyridine)
RN 148099-98-3 CAPLUS
CN Manganese, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)

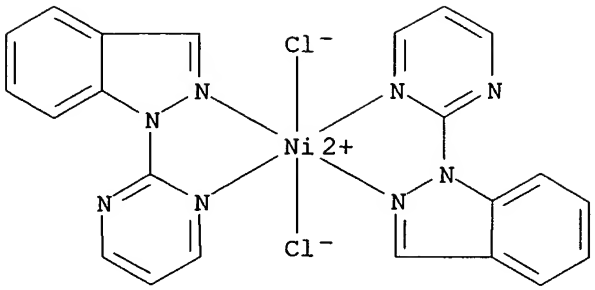


RN 148099-99-4 CAPLUS
CN Cobalt, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)

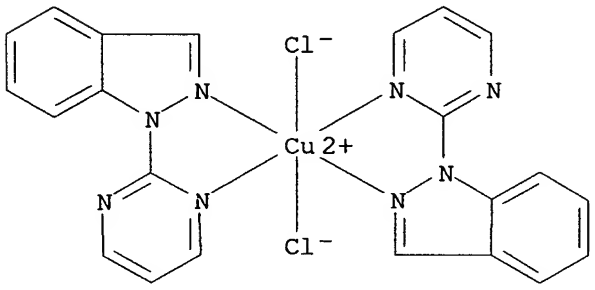


RN 148100-20-3 CAPLUS
CN Nickel, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA

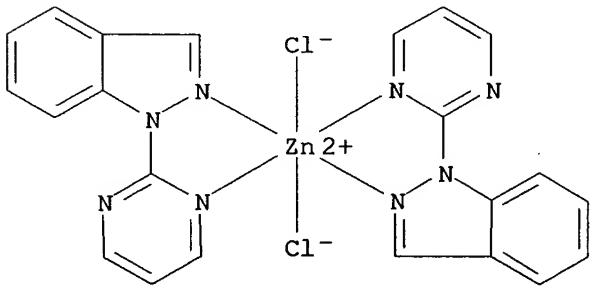
INDEX NAME)



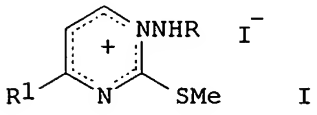
IT **148100-21-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR and UV spectra and reaction of, with pyridine)
RN 148100-21-4 CAPLUS
CN Copper, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)



IT **148100-22-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and IR spectrum and reaction of, with pyridine)
RN 148100-22-5 CAPLUS
CN Zinc, dichlorobis[1-(2-pyrimidinyl)-1H-indazole-NN1,N2]- (9CI) (CA INDEX NAME)



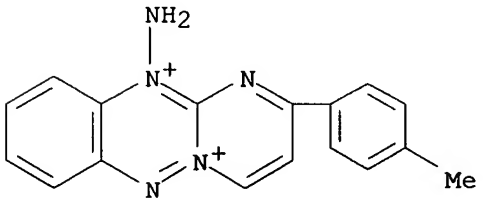
L4 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:235255 CAPLUS
DOCUMENT NUMBER: 112:235255
TITLE: 1-Amino-2-hydrazinopyrimidine N-ylides. Unusual tautomers of 1-aminopyrimidine 2-hydrazones
AUTHOR(S): Liebscher, Juergen; Hassoun, Ahmed; Fabian, Juergen
CORPORATE SOURCE: Sekt. Chem., Humboldt-Univ. Berlin, Berlin, DDR-1040, Ger. Dem. Rep.
SOURCE: Monatshefte fuer Chemie (1989), 120(8-9), 749-58
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:235255
GI



I

AB 1-Amino-2-methylthiopyrimidinium iodides I [R = Ph, COPh, 4-O2NC6H4, 2,4-(O2N)2C6H3, Ac; R1 = Ph, 4-MeC6H4, 4-ClC6H4, 4-MeOC6H4] were prepared by reaction of 3-isothiocyanato-2-propeniminium perchlorates with hydrazines and subsequent methylation of the resulting 1-amino-2(1H)-pyrimidinethiones. Reaction of I with hydrazine causes substitution of the methylthio group and results in the formation of deeply colored 1-amino-2-hydrazinopyrimidine N-ylides as unusual tautomers of the commonly expected 1-amino-2(1H)-pyrimidine hydrazones. The structure of these N-ylides was proved by spectroscopic methods as well as by subsequent transformation to 3-amino-1,2,4-triazole[2,3-a]pyrimidinium salts by dehydration or to pyrimidotriazinium salt by oxidation Reaction of N,N-disubstituted 1-amino-2-methylthiopyrimidinium salt with hydrazine also causes substitution of methylthiol; the resulting orange N,N-disubstituted 1-amino-2(1H)-pyrimidine hydrazone, however, cannot tautomerize to N-ylides.

IT **127252-20-4P 127252-22-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 127252-20-4 CAPLUS
CN Pyrimido[1,2-b][1,2,4]benzotriazin-5-ium, 11-amino-2-(4-methylphenyl)-, dibromide (9CI) (CA INDEX NAME)

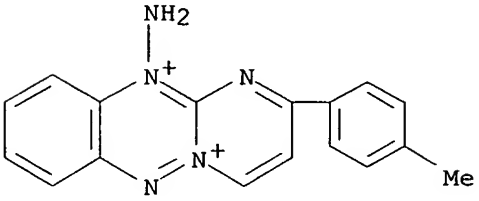


●2 Br⁻

RN 127252-22-6 CAPLUS
CN Pyrimido[1,2-b][1,2,4]benzotriazin-5-ium, 11-amino-2-(4-methylphenyl)-, diperchlorate (9CI) (CA INDEX NAME)

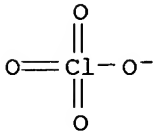
CM 1

CRN 127252-21-5
CMF C17 H15 N5

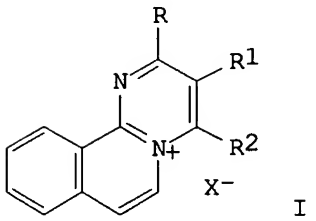


CM 2

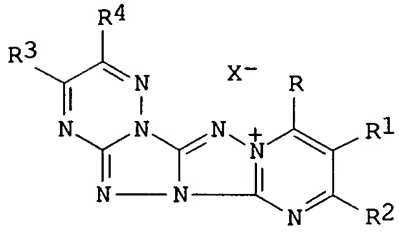
CRN 14797-73-0
CMF Cl O4



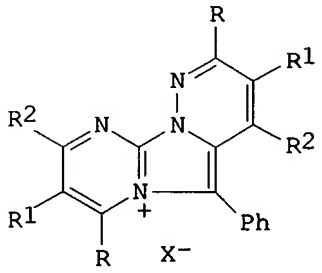
L4 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:544683 CAPLUS
DOCUMENT NUMBER: 85:144683
TITLE: Condensed pyrimidinium salts derived from isoquinoline, condensed s-triazoles, and imidazole
AUTHOR(S): Nuiguk, V. A.; Golubushina, G. M.; Bachkovskii, I. P.; Fedotov, K. V.
CORPORATE SOURCE: Kiev. Univ. im. Shevchenko, Kiev, USSR
SOURCE: Tezisy Dokl. - Simp. Khim. Tekhnol. Geterotsikl. Soedin. Goryuch. Iskop., 2nd (1973), 17-18. Donetsk. Gos. Univ.: Donetsk, USSR.
CODEN: 33XLA8
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



I



II



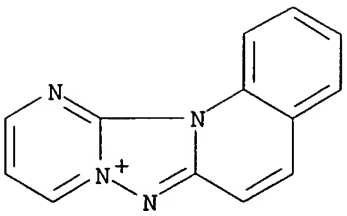
III

AB Condensation of 1-aminoisoquinoline-HClO4 [53686-45-6] with RCOCHR1COR2 or the related β-chlorovinyl ketones gave I. Analogous reactions with 1-amino-s-triazolo[4,3-a]quinoline [41569-09-9], 3-amino-s-triazolo[4,3-b]pyridazine [53854-45-8], or 3-amino-s-triazolo[3,4-a]phthalazine [21517-08-8] gave the resp. condensed pyrimidinium salts. Condensation of 3,6,7-triamino-7H-s-triazolo[4,3-b]-s-triazole [13728-15-9] with RCOCHR1COR2 and R3COCOR4 gave II via the intermediates with only 1 ring added. Condensation of 1,2-diamino-4-phenylimidazole [15970-40-8] with 2 moles RCOCHR1COR2 gave III. Any of these condensed pyrimidinium salts with R, R1, or R2 = Me could be converted to cyanines.

IT **54063-69-3DP**, Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 54063-69-3 CAPLUS

CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium (9CI) (CA INDEX NAME)


N
N
N+
N

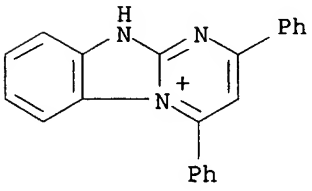
L4 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:74304 CAPLUS
DOCUMENT NUMBER: 84:74304
TITLE: 1,3-Diphenylpyrimido[1,2:a]benzimidazolium perchlorates
INVENTOR(S): Zvezdina, E. A.; Dorofeenko, G. N.; Zhdanova, M. P.; Simonov, A. M.
PATENT ASSIGNEE(S): Rostov State University, USSR
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1975, 52(41), 97.
CODEN: URXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Russian
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
SU 490801	T	19751105	SU 1974-1993642		19740129
PRIORITY APPLN. INFO.:			SU 1974-1993642	A	19740129

GI For diagram(s), see printed CA Issue.
AB The title compds. I (R = lower alkyl or aralkyl; R1 = H, Me) were prepared by treatment of 2-aminobenzimidazoles with 2,4,6-triphenylpyrylium perchlorate in absolute DMF at reflux.
IT **58537-58-9DP**, 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-diphenyl-, perchlorate, derivs. **58537-60-3DP**, 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 7,8-dimethyl-2,4-diphenyl-, perchlorate, derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 58537-58-9 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-diphenyl-, perchlorate (9CI) (CA INDEX NAME)

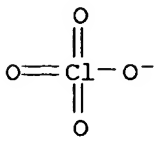
CM 1

CRN 58537-57-8
CMF C22 H16 N3



CM 2

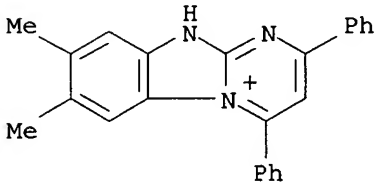
CRN 14797-73-0
CMF Cl O4



RN 58537-60-3 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 7,8-dimethyl-2,4-diphenyl-, perchlorate (9CI) (CA INDEX NAME)

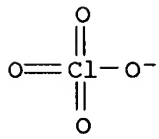
CM 1

CRN 58537-59-0
CMF C24 H20 N3

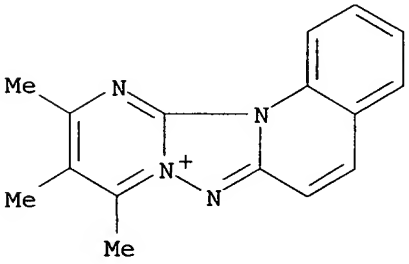


CM 2

CRN 14797-73-0
CMF Cl O4

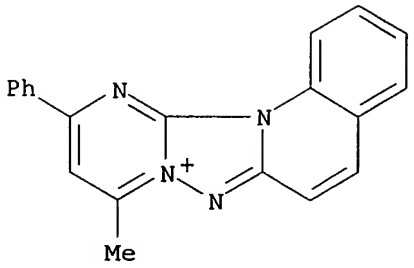


L4 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:552154 CAPLUS
DOCUMENT NUMBER: 81:152154
TITLE: New heterocyclic systems of S-triazolopyrimidinium derivatives of quinoline, pyridazine, and phthalazine
AUTHOR(S): Golubushina, G. M.; Ponomarenko, O. G.; Poshtaruk, G. N.; Chuiguk, V. A.
CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1974), (6), 843-5
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Pyrimido-triazolopyridazinium perchlorates (I; R1 = H, Cl, R2 = H, Me; R3 = Me, H; R4 = Me, Ph, H) were obtained in 39-100% yields by condensation of a β-diketone with an aminotriazolopyridazine in F3CCO2H. Analogously obtained were 63-100% II (R1 = Me, Ph, H, R2 = H, Me, R3 = Me, H) and 80-5% III (R1 = Me, Ph; R2 = H, Me; R3 = Me; X = ClO4, iodo, Br) in the absence of solvent.
IT **53854-43-6P 53854-44-7P 53890-38-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 53854-43-6 CAPLUS
CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, 9,10,11-trimethyl-, iodide (9CI) (CA INDEX NAME)



● I⁻

RN 53854-44-7 CAPLUS
CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, 9-methyl-11-phenyl-, bromide (9CI) (CA INDEX NAME)

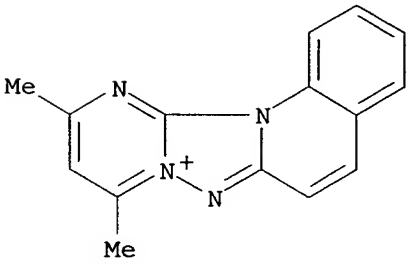


● Br^-

RN 53890-38-3 CAPLUS
CN Pyrimido[1',2':1,5][1,2,4]triazolo[4,3-a]quinolin-8-ium, 9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

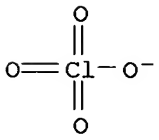
CM 1

CRN 53890-37-2
CMF C15 H13 N4



CM 2

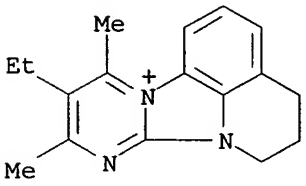
CRN 14797-73-0
CMF Cl O4



L4 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:488425 CAPLUS
DOCUMENT NUMBER: 77:88425
TITLE: Condensation of 2-amino-3,4,5,6-tetrahydroimidazo [4,5,1-ij]quinoline and 2-amino-2-pyrrline with β-diketones
AUTHOR(S): Golubushina, G. M.; Chuiguk, V. A.
CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1972), (3), 419-21
CODEN: KGSSAQ; ISSN: 0132-6244
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB 2-Amino-3,4,5,6-tetrahydroimidazo[4,5,1-ij]-quinoline perchlorate when heated 2 hr at 180-90° with β-diketones gave five 1,2,3,12-tetrahydropyrimido[2 , 1 :2,3]imidazo-[4,5,1-ij]quinolinium perchlorates (I, R, R1, R2 = H, Me, Ph, Et) in yields of 18-58%. 4-Methyl-7,8-dihydro-6H-pyrrolo[1,2-a]pyrimidinium perchlorates (II, R = Me, Ph) were similarly prepared in 20-27% yield.
IT **38340-23-7P 38340-24-8P 38340-70-4P 38340-71-5P 38340-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38340-23-7 CAPLUS
CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 10-ethyl-5,6-dihydro-9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

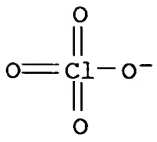
CM 1

CRN 47045-38-5
CMF C17 H20 N3



CM 2

CRN 14797-73-0
CMF Cl O4

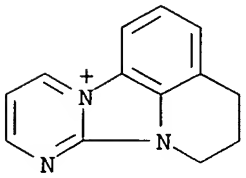


RN 38340-24-8 CAPLUS

CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-, perchlorate (9CI) (CA INDEX NAME)

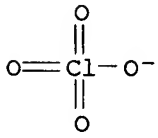
CM 1

CRN 46487-03-0
CMF C13 H12 N3



CM 2

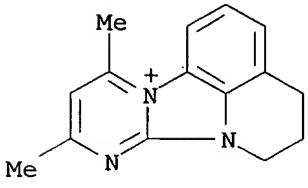
CRN 14797-73-0
CMF Cl O4



RN 38340-70-4 CAPLUS
CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-9,11-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

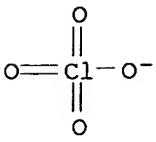
CM 1

CRN 46864-77-1
CMF C15 H16 N3



CM 2

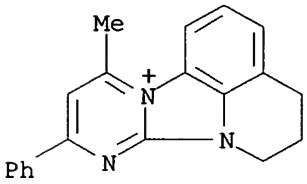
CRN 14797-73-0
CMF Cl O4



RN 38340-71-5 CAPLUS
CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-11-methyl-9-phenyl-, perchlorate (9CI) (CA INDEX NAME)

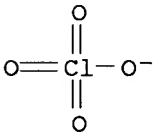
CM 1

CRN 47286-43-1
CMF C20 H18 N3



CM 2

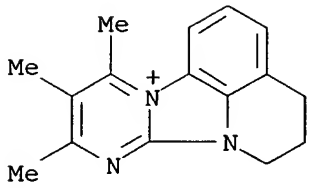
CRN 14797-73-0
CMF Cl O4



RN 38340-72-6 CAPLUS
CN 4H-Pyrimido[2',1':2,3]imidazo[4,5,1-ij]quinolin-12-ium, 5,6-dihydro-9,10,11-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

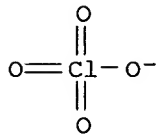
CM 1

CRN 46960-85-4
CMF C16 H18 N3



CM 2

CRN 14797-73-0
CMF Cl O4



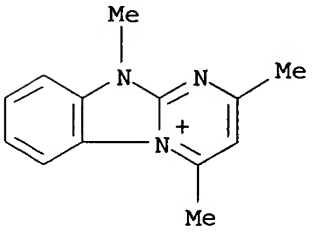
L4 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:59508 CAPLUS
DOCUMENT NUMBER: 76:59508
TITLE: Synthesis and pharmacological properties of some new condensed derivatives of benzothiazoline thiazolo, and benzothiazolopyrimidine
AUTHOR(S): Lisunkin, Yu. I.; Chuiguk, V. A.
CORPORATE SOURCE: Kiev Res. Inst. Pharmacol. Toxicol., Kiev, USSR
SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1971), 26(5), 20-5
CODEN: FRZKAP; ISSN: 0367-3057
DOCUMENT TYPE: Journal
LANGUAGE: Ukrainian

AB 2-Amino- and 1-methyl-2-amino-2-imidazoline-HBr and -thiazole-HBr, 2-amino-4-phenylthiazole-HBr, 2-aminobenzothiazole-HBr, and 1-methyl-2-aminobenzimidazole-HBr condensed with Ac2CH2 to give the corresponding condensed-ring heterocyclic pyrimidinium salts in 39-95% yield. 3a,9-Dimethyl- and 3a-methyl-1,2,3,3a-tetrahydropyrrolo[2,1-b]benzothiazolium chloride and 4a-methyl-1,2,3,4,4a,10-hexahydro[2,1-b]benzothiazolium and -benzoxazolium bromide were prepared analogously using 0-H2NC6H6OH and 0-H2NC6H4SH derivs. These compds. exerted a hypotensive effect when administered i.v. to mice, but did not affect pain sensitivity or the duration of barbiturate or chloral hydrate narcosis; LD50 values were 38-385 mg/kg body weight Arecoline and nicotine hyperkinesis in mice were ptentiated; the sensitivity of frog transverse abdominal muscle to acetylcholine was reduced.

IT **35220-93-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35220-93-0 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4,10-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

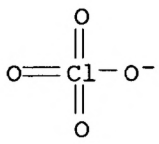
CM 1

CRN 46496-90-6
CMF C13 H14 N3



CM 2

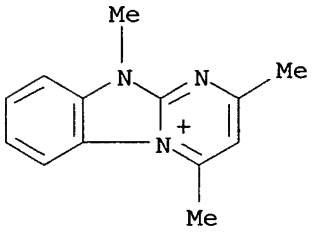
CRN 14797-73-0
CMF Cl O4



L4 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:46158 CAPLUS
DOCUMENT NUMBER: 76:46158
TITLE: Condensation of salts of 2-aminobenzimidazoles with β-diketones and β-chlorovinyl ketones
AUTHOR(S): Golubushina, G. M.; Chuiguk, V. A.
CORPORATE SOURCE: Kiev. Gos. Univ. im. Shevchenko, Kiev, USSR
SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (1971), 37(11), 1132-4
CODEN: UKZHAU; ISSN: 0041-6045
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Salts of 2-amino-1-methyl- and 2-amino-1-phenylbenzimidazole were condensed with β-diketones and β-chlorovinyl ketones to form 8 quaternary salts of structure I (R=Me or Ph, R1 and R3=H or Me, and R2=Me, Et, or Ph). Some of these compds. were identical with the quaternary salts obtained from pyrimido[1,2-a]benzimidazoles (CA 59: 15411c) which indicates that the latter do not have structure II.
IT **35220-93-0P 35220-95-2P 35220-96-3P 35220-97-4P 35220-98-5P 35220-99-6P 35221-00-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35220-93-0 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4,10-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

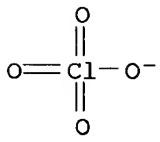
CM 1

CRN 46496-90-6
CMF C13 H14 N3



CM 2

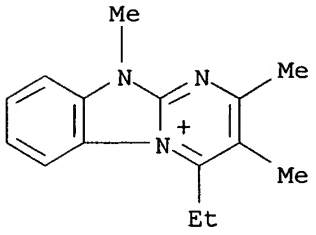
CRN 14797-73-0
CMF Cl O4



RN 35220-95-2 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-ethyl-2,3,10-trimethyl-, perchlorate (9CI) (CA INDEX NAME)

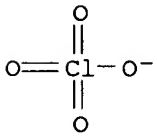
CM 1

CRN 46864-34-0
CMF C15 H18 N3



CM 2

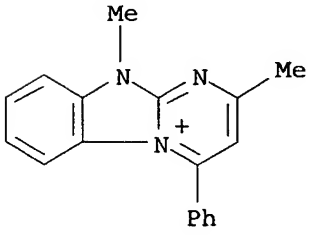
CRN 14797-73-0
CMF Cl O4



RN 35220-96-3 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,10-dimethyl-4-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

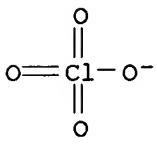
CRN 47127-07-1
CMF C18 H16 N3



CM 2

CRN 14797-73-0

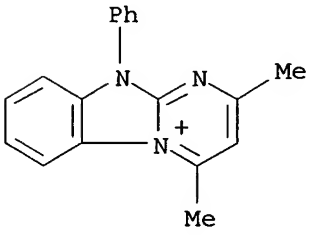
CMF Cl O4



RN 35220-97-4 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 2,4-dimethyl-10-phenyl-, salt with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

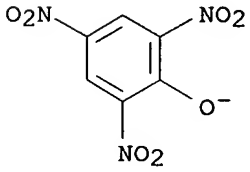
CM 1

CRN 47127-37-7
CMF C18 H16 N3



CM 2

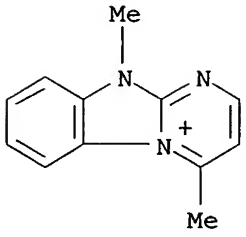
CRN 14798-26-6
CMF C6 H2 N3 O7



RN 35220-98-5 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4,10-dimethyl-, perchlorate (9CI) (CA INDEX NAME)

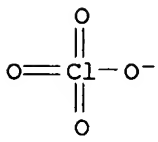
CM 1

CRN 46388-80-1
CMF C12 H12 N3



CM 2

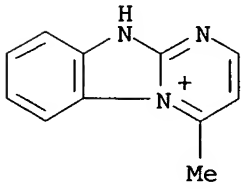
CRN 14797-73-0
CMF Cl O4



RN 35220-99-6 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-methyl-, perchlorate (9CI) (CA INDEX NAME)

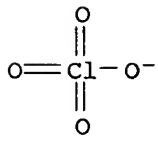
CM 1

CRN 46266-98-2
CMF C11 H10 N3



CM 2

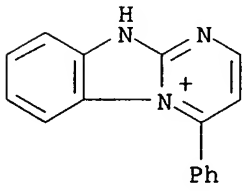
CRN 14797-73-0
CMF Cl O4



RN 35221-00-2 CAPLUS
CN 10H-Pyrimido[1,2-a]benzimidazol-5-ium, 4-phenyl-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 46955-67-3
CMF C16 H12 N3



CM 2

CRN 14797-73-0
CMF Cl O4